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NONLINEAR INTEGRAL EQUATIONS OF RADIATIVE TRANSFER*

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NONLINEAR INTEGRAL EQUATIONS OF RADIATIVE TRANSFER

1. INTRODUCTION

The area of mathematical physics which we shall discuss is somewhat unique compared to the others discussed in this seminar. A peculiar feature of this subject is the fact that within the mathematical model of certain radiative transfer problems there are both linear and nonlinear equations which determine desired functions. As opposed to the usual situation, the linear equations are exact and not merely linear approximations to the nonlinear equations. This fortunate situation permits us to obtain many exact results about the nonlinear equations by a study of the linear equations.

We shall discuss one of the relatively simple problems in the theory of radiative transfer; that of determining quantitatively the intensity of radiation (neglecting polarization and redistribution of absorbed radiation) in a homogeneous, plane-parallel atmosphere that is of finite thickness and infinite lateral extent, and that is exposed to monochromatic radiation impinging on one side of the atmosphere from a given direction. This also describes the transport of monoenergetic neutrons in a sub-critical slab reactor.

The mathematical formulation of this problem as a scalar linear integro-differential equation dates back to Schwarzschild [64,65] and has been extensively studied

[Cf. 16, 21, 30, 33, 34, 36, 38, 39, 46, 47, 78]. If a steady state prevails, boundary conditions on the face of the atmosphere allow the conversion to a linear integral equation. This equation is solved uniquely by a series, the n -th term of which gives the contribution of radiation which has been scattered n times [Cf. 34].

In theory then this problem is completely solved. The actual computation of quantities by means of the series is practical, however, only if either the atmosphere is thin or absorption is strong for each scattering. It is in an attempt to find more practical methods of computation that various authors have formulated nonlinear equations.

Most astronomical observations give only radiation reflected from or transmitted through an atmosphere, whereas the above mentioned solution to the transport equation gives a solution throughout the atmosphere. This led Ambarzumian first to the formulation of nonlinear integral equations for the intensity of radiation reflected from a semi-infinite atmosphere [1]. These equations were derived by observing that the problem for a semi-infinite atmosphere is invariant under the addition of a slab of finite thickness. This idea has been exploited by Ambarzumian [4] and Sobolev [68, 69], by Chandrasekhar [22, 23] under the name of "Principles of Invariance," and by Preisendorfer [58-60], Bellman, Kalaba, and Wing [11-13], Redheffer [62, 63], Ueno [75, 76], and others under the title of "Invariant Imbedding." Many of the derivations of these equations

have been heuristic and are similar to the standard heuristic method for deriving equations in mathematical physics by particle counting, being novel in that the physical parameter of atmospheric thickness is varied.

It is easily shown that these nonlinear equations can be derived rigorously from the transport equation [8, 9, 16, 36, 49]. For more complicated geometries this seems preferable since the heuristic particle counting has lead to errors [9].

We shall sketch below the derivation of some of these nonlinear equations from the transport equation. We shall also show that the same functions can be obtained as solutions to linear singular integral equations. With these linear equations it is possible to do precise existence and uniqueness studies.

For the sake of simplicity we shall restrict ourselves to the case of isotropic scattering. In this case some of the derivations are deceptively simple. The results which we shall give can be extended to anisotropic scattering, and we shall give references where appropriate. For certain well known results, which are derived in a new manner, the method of derivation is given since it is the one most easily extended to anisotropic scattering.

We do not attempt to give any part of the theories of polarization [22], of inhomogeneous media [13, 19, 49, 74] or of other geometries (8, 13, 22, 59] and other boundary value problems [23]. We do not touch on the problems of

neutron reactor theory, which fit naturally into this subject matter but in which one often asks different questions than those considered here. Neither do we consider various numerical methods obtained by replacing the linear transport equation by a system of approximate equations [4, 6, 7, 20, 22, 71].

In summary then our objective is to take the simplest problem which is of physical significance and which will serve to display the derivations and useful role of certain formulations other than the transport equation. Of particular importance are the questions of existence, uniqueness, and practicality for computational purposes.

We give a list of references which is extensive but by no means exhaustive. Additional references can be found in many of the papers and books cited, and no slight is meant here by the omission of references to any particular author or work.

2. THE TRANSPORT EQUATION

We shall consider a homogeneous plane-parallel atmosphere of finite optical thickness τ . Optical depth into the medium is measured by a variable x , $0 \leq x \leq \tau$, in a direction normal to a face of the atmosphere. We let $I(x, \mu, \phi)$ denote intensity of radiation at depth x in a direction specified by θ , the inclination to the positive x axis, and by ϕ , the azimuth referred to a fixed axis normal to the x axis. Here $\mu = \cos \theta$.

The notion of homogeneity should perhaps be clarified. An actual atmosphere can have variations in the density and in the mass absorption and scattering coefficients [22]. The optical depth is introduced as a variable to remove these variations from the equation. If after this transformation of variables the law of local scattering is constant, the medium is said to be homogeneous.

The interaction of radiation with the medium results in absorption as well as the scattering of some of this energy into other directions. We shall assume that radiation fields do not interact with each other, that the frequency of the radiation is unchanged upon scattering, and that absorbed radiation is not reemitted.

We consider a monochromatic parallel beam of radiation of unit average intensity per unit time falling on the entire face of the atmosphere at $x = 0$ from some direction (ψ, ϕ) . We suppose that a steady state exists. Rather

than formulate the incident field as a boundary condition in the form of a δ -function in direction, we consider the reduced incident field as a source throughout the medium. If we consider isotropic scattering, the transport equation for the intensity of diffuse radiation is independent of ϕ and is given by [22, 34],

$$(2.1) \quad \mu \frac{\partial I}{\partial x}(x, \mu, \nu) + I(x, \mu, \nu) = J(x, \nu),$$

where the source function J is given by

$$(2.2) \quad J(x, \nu) = \exp[-x/\nu] + \frac{\omega}{2} \int_{-1}^1 I(x, \sigma, \nu) d\sigma,$$

$$0 \leq \omega \leq 1, \quad -1 \leq \mu \leq 1, \quad 0 \leq \nu \leq 1.$$

If we consider the medium surrounding the atmosphere as a vacuum, then no diffuse radiation enters the faces of the atmosphere. This gives the boundary conditions

$$(2.3) \quad I(0, \mu, \nu) = I(\tau, -\mu, \nu) = 0, \quad 0 \leq \mu \leq 1.$$

We have given the transport equation for isotropic scattering. The results to be given below have extensions to the case of anisotropic scattering where ω in (2.2) is replaced under the integral by a phase function which is usually assumed to be given by a finite expansion in

Legendre polynomials of the cosine of the angle between incident and observational directions [c.f. 22, 34].

Using the boundary conditions (2.3), we have from (2.1)

$$(2.4) \quad I(x, \mu, \nu) = \frac{1}{\mu} \int_0^x \exp[(y-x)/\mu] J(y, \nu) dy$$

for $0 < \mu \leq 1$, and

$$(2.5) \quad I(x, \mu, \nu) = \frac{1}{|\mu|} \int_x^\tau \exp[(y-x)/\mu] J(y, \nu) dy$$

for $-1 \leq \mu < 0$.

If these relations are inserted in (2.2) we obtain the familiar linear integral equation [22, 34]

$$(2.6) \quad J(x, \nu) = \exp[-x/\nu] + \frac{\omega}{2} \int_0^1 \int_0^\tau \exp[-|x-y|/\mu] J(y, \nu) dy \frac{d\mu}{\mu}$$

The integral operator without ω is known as the truncated Hopf operator Λ and it has been intensively studied [20, 30, 34, 38, 39, 50, 78]. This operator is usually written in terms of the exponential integral $E_1(x)$, but for later computational purposes we prefer the above form.

For the physical application it is the solution of (2.6) for ν in the interval $0 \leq \nu \leq 1$ that is of importance. For the mathematical analysis that follows it is important to consider solutions for all nonzero complex values of ν . We shall state the following

Legendre polynomials of the cosine of the angle between incident and observational directions [c.f. 22, 34].

Using the boundary conditions (2.3), we have from (2.1)

$$(2.4) \quad I(x, \mu, \nu) = \frac{1}{\mu} \int_0^x \exp[(y - x)/\mu] J(y, \nu) dy$$

for $0 < \mu \leq 1$, and

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well-known theorem [16, 34, 36] which has an appropriate extension to anisotropic scattering.

Theorem 1. For $0 \leq \omega \leq 1$ and $0 \leq \tau < \infty$ the
equation

$$(2.7) \quad J - \omega \Lambda(J) = B$$

has a unique solution for any bounded function B given
by

$$(2.8) \quad J = \sum_{n=0}^{\infty} \omega^n \Lambda^n(B).$$

If for $|\nu| > 0$, we take

$$(2.9) \quad B = \exp[-x/\nu],$$

then J is analytic in the extended domain $|\nu| > 0$
and real valued and nonnegative for real $\nu \neq 0$.

This is the basic existence and uniqueness result which expresses the solution in familiar terms as the sum of contributions from n-th order scatterings. The series (2.8) converges geometrically with a ratio equal to ω times the maximum eigenvalue $\lambda(\tau)$ of Λ . Many estimates of λ as a function of τ have been made [c.f. 20, 50]. Since λ is asymptotic to 1 as τ goes to infinity, e.g., $\lambda(4) = .9$, the series computation is practical

only for small τ or for small ω .

Our objective below is to discuss other formulations that replace (2.7) by other equations and replace (2.8) by a computation which is practical for all $0 \leq \tau < \infty$ and $0 \leq \omega \leq 1$.

3. NONLINEAR EQUATIONS

We now derive certain nonlinear equations for determining I and J on the faces of the atmosphere. One motivation for this is that the computation of I throughout the atmosphere represents unnecessary work for many applications since it is only the reflected or transmitted intensities that are observed (p. 555 of [3]). Another motivation is the fact that the outward intensities on the faces of the atmosphere represent missing boundary conditions for the transport equation. If these boundary conditions can be determined then it is a simple matter to compute intensities interior.

Many of the derivations of nonlinear equations are heuristic arguments based on "Principles of Invariance" [3, 22] or the "Principle of Invariant Imbedding" [13, 76]. We shall not state any of these principles but instead sketch a derivation of the nonlinear equations from the transport equation.

We first define certain standard functions. The scattering function S and the transmission function T are defined by [22]

$$\begin{aligned} S(\mu, \nu) &= \mu I(0, -\mu, \nu), \\ (3.1) \quad T(\mu, \nu) &= \mu I(\tau, \mu, \nu), \quad 0 \leq \mu \leq 1. \end{aligned}$$

By (2.4) and (2.5) these are merely Laplace transforms of the function J which is defined to be zero outside the interval $0 \leq x \leq \tau$, that is

$$\begin{aligned} S(\mu, \nu) &= \int_0^{\tau} \exp[-y/\mu] J(y, \nu) dy, \\ T(\mu, \nu) &= \int_0^{\tau} \exp[-(\tau-y)/\mu] J(y, \nu) dy. \end{aligned} \quad (3.2)$$

These functions are well defined in the complex μ -plane, $|\mu| > 0$, as entire functions of the variable μ^{-1} . In this setting they are dependent since

$$(3.3) \quad S(\mu, \nu) = \exp[-\tau/\mu] T(-\mu, \nu).$$

In view of our previous comment on analyticity of J in ν , S and T are analytic in μ and ν for all $|\mu| > 0$ and $|\nu| > 0$.

Following Busbridge [16], we define X and Y functions by

$$\begin{aligned} X(\mu) &= J(0, \mu), \\ Y(\mu) &= J(\tau, \mu). \end{aligned} \quad (3.4)$$

From (2.6) it is obvious that

$$(3.5) \quad J(\tau - x, \mu) = \exp[-\tau/\mu] J(x, -\mu)$$

so that

$$(3.6) \quad Y(\mu) = \exp[-\tau/\mu]X(-\mu).$$

Using (3.2) and (3.4) in (2.6) we see also that

$$(3.7) \quad \begin{aligned} X(\mu) &= 1 + \frac{\omega}{2} \int_0^1 S(\sigma, \mu) \frac{d\sigma}{\sigma}, \\ Y(\mu) &= \exp[-\tau/\mu] + \frac{\omega}{2} \int_0^1 T(\sigma, \mu) \frac{d\sigma}{\sigma}. \end{aligned}$$

By the definition of S and T and the self-adjointness of the operator Λ , we have

$$(3.8) \quad \begin{aligned} S(\mu, \nu) &= S(\nu, \mu), \\ T(\mu, \nu) &= T(\nu, \mu). \end{aligned}$$

This fact is also true for anisotropic scattering [3, 22, 52], but the proof is more complicated since the operator replacing Λ in general is not self-adjoint [52].

A differentiation of equation (2.6) gives by Theorem 1 the following theorem [16, 22].

Theorem 2. Let J satisfy (2.6). Then for
 $0 < x < \tau$ we have

$$(3.9) \quad \frac{\partial J}{\partial x}(x, \mu) + \mu^{-1} J(x, \mu) = \frac{\omega X(\mu)}{2} \int_0^1 J(x, \sigma) \frac{d\sigma}{\sigma} - \frac{\omega Y(\mu)}{2} \int_0^1 J(\tau - x, \sigma) \frac{d\sigma}{\sigma}.$$

For $0 \leq x < \tau$, the onesided derivative $\frac{\partial J}{\partial \tau}$ is given by

$$(3.10) \quad \frac{\partial J}{\partial \tau}(x, \mu) = \frac{\omega}{2} Y(\mu) \int_0^1 J(\tau - x, \sigma) \frac{d\sigma}{\sigma}.$$

This theorem has an appropriate extension to anisotropic scattering [52].

If we multiply (3.9) by $\exp(-x/\nu)$ and $\exp[-(\tau-x)/\nu]$ and integrate, we obtain the familiar equations [16, 22]

$$(3.11) \quad \begin{aligned} \left(\frac{1}{\mu} + \frac{1}{\nu}\right) S(\mu, \nu) &= X(\mu)X(\nu) - Y(\mu)Y(\nu), \\ \left(\frac{1}{\mu} - \frac{1}{\nu}\right) T(\mu, \nu) &= X(\mu)Y(\nu) - Y(\mu)X(\nu). \end{aligned}$$

If these are inserted in (3.7) we obtain Chandrasekhar's equations for $0 \leq \mu \leq 1$,

$$(3.12) \quad \begin{aligned} X(\mu) &= 1 + \frac{\mu\omega}{2} \int_0^1 \frac{X(\mu)X(\nu) - Y(\mu)Y(\nu)}{\mu + \nu} d\nu, \\ Y(\mu) &= \exp[-\tau/\mu] + \frac{\mu\omega}{2} \int_0^1 \frac{Y(\mu)X(\nu) - X(\mu)Y(\nu)}{\mu - \nu} d\nu. \end{aligned}$$

If (3.10) is substituted in (3.9) and the Laplace transforms taken, we obtain the familiar equations [22]

$$\begin{aligned}
 & \left(\frac{1}{\mu} + \frac{1}{\nu} \right) S(\mu, \nu) + \frac{\partial S}{\partial \tau} (\mu, \nu) \\
 & = \left[1 + \frac{\omega}{2} \int_0^1 S(\mu, \sigma) \frac{d\sigma}{\sigma} \right] \left[1 + \frac{\omega}{2} \int_0^1 S(\nu, \sigma) \frac{d\sigma}{\sigma} \right], \\
 (3.13) \quad & \frac{1}{\mu} T(\mu, \nu) + \frac{\partial T}{\partial \tau} (\mu, \nu) \\
 & = \left[1 + \frac{\omega}{2} \int_0^1 S(\mu, \sigma) \frac{d\sigma}{\sigma} \right] \left[e^{-\tau/\nu} + \frac{\omega}{2} \int_0^1 T(\nu, \sigma) \frac{d\sigma}{\sigma} \right].
 \end{aligned}$$

Equation (3.10) is also useful in obtaining an instability result discussed in Sec. 6. Setting $x = 0$ we obtain [22]

$$(3.14) \quad \frac{\partial X}{\partial \tau} (\mu, \tau) = Y(\mu, \tau) \frac{\omega}{2} \int_0^1 Y(\sigma, \tau) \frac{d\sigma}{\sigma}, \quad \tau > 0.$$

Using this and (3.6) we get [22]

$$(3.15) \quad \frac{\partial Y}{\partial \tau} (\mu, \tau) + \frac{1}{\mu} Y(\mu, \tau) = X(\mu, \tau) \frac{\omega}{2} \int_0^1 Y(\sigma, \tau) \frac{d\sigma}{\sigma}, \quad \tau > 0.$$

Analogous definitions and results have been given for anisotropic scattering [22, 52]. For isotropic scattering problems in other geometries, Bailey [8] and Bailey and Wing [9] have given similar rigorous derivations of invariance principles from the transport equation. One

interesting feature of this work is the disclosure of an error in previous heuristic derivations [9].

Equations (3.12) and (3.13) are the nonlinear equations which have been most used for numerical calculations [14, 24, 25, 26, 27, 28, 41]. They represent necessary conditions only on the solution J to (2.6) [22]. Before considering the important questions of uniqueness and stability, we turn in the next section to the derivation of certain linear equations which are also necessary conditions on S , T , X , and Y .

4. LINEAR SINGULAR EQUATIONS

We want now to derive certain linear equations as necessary conditions on the unique solution J to equation (2.6). For the isotropic case a derivation of these equations from the nonlinear X and Y equations is due to Busbridge [16, 36]. (See also Crum [29].) Busbridge's approach has never been extended to similar equations for anisotropic scattering. For this reason we give a different derivation for the isotropic case which does readily extend to the anisotropic case [54].

We apply the operator Λ to equation (2.6). With Λ expressed as in (2.6), it is an easy computation to show that for v replaced by any complex number z outside the interval $[-1, 1]$ we have the equation for $\Lambda(J)$

$$\begin{aligned}
 (4.1) \quad \omega \Lambda(J)(x, z) - (\omega \Lambda)^2(J)(x, z) &= \frac{z\omega}{2} \exp[-x/z] \int_{-1}^1 \frac{d\sigma}{z-\sigma} \\
 &- \frac{z\omega}{2} \int_0^1 \frac{\exp[-x/\sigma]}{z-\sigma} d\sigma \\
 &- \frac{z\omega}{2} \exp[-\tau/z] \int_0^1 \frac{\exp[-(\tau-x)/\sigma]}{z+\sigma} d\sigma.
 \end{aligned}$$

By the uniqueness result of Theorem 1, we obtain the solution

$$(4.2) \quad \omega \lambda(J)(x, z) = J(x, z) \frac{zw}{2} \int_{-1}^1 \frac{d\sigma}{z-\sigma} - \frac{zw}{2} \int_0^1 \frac{J(x, \sigma)}{z-\sigma} d\sigma \\ - \frac{zw}{2} \exp[-\tau/z] \int_0^1 \frac{J(\tau-x, \sigma)}{z+\sigma} d\sigma .$$

The last term follows from (3.5).

Combining this with (2.6) we obtain linear conditions on J .

Theorem 3. For complex z outside the interval $[-1, 1]$ the unique solution to (2.6) also satisfies the equation

$$(4.3) \quad \lambda(z)J(x, z) = \exp[-x/z] - \frac{zw}{2} \int_0^1 \frac{J(x, \sigma)}{z-\sigma} d\sigma \\ - \frac{zw}{2} \exp(-\tau/z) \int_0^1 \frac{J(\tau-x, \sigma)}{z+\sigma} d\sigma .$$

The function λ is defined by

$$(4.4) \quad \lambda(z) = 1 - \frac{zw}{2} \int_{-1}^1 \frac{d\sigma}{z-\sigma} ,$$

and x is merely a parameter satisfying $0 \leq x \leq \tau$.

If $J(x, \mu)$ and $J(\tau-x, \mu)$ are known for $0 \leq \mu \leq 1$, then (4.3) defines their meromorphic extension to complex z outside $[-1, 1]$. If J is to satisfy (2.6), it must be analytic in all z for $|z| > 0$. This means that

the right hand side of (4.3) must vanish at the zeros of λ .

The function λ is even and has only two real roots. For $0 \leq w < 1$ these are given by $\pm 1/k$ where k is the nonzero root of

$$(4.5) \quad 2k = w \ln \frac{1+k}{1-k}.$$

For $w = 1$, λ has a double root at infinity.

We demand that the right hand side of (4.3) vanish to the same order as λ . For $0 \leq w < 1$ we obtain the conditions

$$(4.6) \quad \exp[\pm kx] = \frac{w}{2} \int_0^1 \frac{J(x, \sigma) d\sigma}{1 \pm k\sigma} + \frac{w}{2} \exp[\pm k\tau] \int_0^1 \frac{J(\tau-x, \sigma) d\sigma}{1 \mp k\sigma}.$$

For $w = 1$, we have

$$(4.7) \quad \begin{aligned} 2 &= \int_0^1 [J(x, \sigma) + J(\tau-x, \sigma)] d\sigma, \\ \tau \int_0^1 J(\tau-x, \sigma) d\sigma &= 2x + \int_0^1 \sigma [J(x, \sigma) - J(\tau-x, \sigma)] d\sigma \end{aligned}$$

We have therefore obtained two linear constraints on J for each x by demanding analyticity in the variable z .

Now we can use Plemelj's formula [57] to obtain singular equations for determining $J(x, \mu)$ and $J(\tau-x, \mu)$ on $0 \leq \mu \leq 1$. For μ in $0 < \mu < 1$ we take limits of (4.3) in the complex plane as z tends to μ first with $\text{Im}(z) > 0$ and then with $\text{Im}(z) < 0$. Adding these limits and using analyticity of J , we obtain the singular equation [54]

$$(4.8) \quad \lambda_0(\mu)J(x, \mu) = \exp[-x/\mu] - \frac{\mu\omega}{2} \int_0^1 \frac{J(x, \sigma)}{\mu-\sigma} d\sigma \\ - \frac{\mu\omega}{2} \exp[-\tau/\mu] \int_0^1 \frac{J(\tau-x, \sigma)}{\mu+\sigma} d\sigma .$$

The singular integrals are computed as Cauchy principle values. The function λ_0 is given by

$$(4.9) \quad \lambda_0(\mu) = 1 + \frac{\mu\omega}{2} \ln \frac{1-\mu}{1+\mu} .$$

If we evaluate (4.8) at $x = 0$ and at $x = \tau$ and recall (3.4) we obtain the equations [16, 29, 31, 53]

$$(4.10) \quad \lambda_0(\mu)X(\mu) = 1 - \frac{\mu\omega}{2} \int_0^1 \frac{X(\sigma)d\sigma}{\mu-\sigma} - \frac{\mu\omega}{2} \exp[-\tau/\mu] \int_0^1 \frac{Y(\sigma)d\sigma}{\mu+\sigma} \\ \lambda_0(\mu)Y(\mu) = \exp[-\tau/\mu] \left[1 - \frac{\mu\omega}{2} \int_0^1 \frac{X(\sigma)d\sigma}{\mu+\sigma} \right] - \frac{\mu\omega}{2} \int_0^1 \frac{Y(\sigma)d\sigma}{\mu-\sigma}$$

If equation (4.3) is multiplied by $\exp[-x/v]$ and by $\exp[-(\tau-x)/v]$ and integrated on x , we obtain the following analogous equations for S and T functions [52]. The linear singular equations are

$$\begin{aligned}
 \lambda_0(\mu)S(v, \mu) &= \frac{\mu v}{\mu+v} \left(1 - \exp\left[-\tau\left(\frac{1}{v} + \frac{1}{\mu}\right)\right]\right) - \frac{\mu w}{2} \int_0^1 \frac{S(v, \sigma) d\sigma}{\mu-\sigma} \\
 &\quad - \frac{\mu w}{2} \exp[-\tau/\mu] \int_0^1 \frac{T(v, \sigma) d\sigma}{\mu+\sigma} \\
 (4.11) \quad \lambda_0(\mu)T(v, \mu) &= \frac{\mu v}{\mu-v} \left(\exp[-\tau/\mu] - \exp[-\tau/v]\right) - \frac{\mu w}{2} \int_0^1 \frac{T(v, \sigma) d\sigma}{\mu-\sigma} \\
 &\quad - \frac{\mu w}{2} \exp[-\tau/\mu] \int_0^1 \frac{S(v, \sigma) d\sigma}{\mu+\sigma}
 \end{aligned}$$

For $0 \leq w < 1$ the linear constraints are

$$\begin{aligned}
 (4.12) \quad \frac{v}{1 \pm kv} \left(1 - \exp\left[-\tau\left(\frac{1}{v} \pm k\right)\right]\right) &= \frac{w}{2} \int_0^1 \frac{S(v, \sigma) d\sigma}{1 \mp k\sigma} \\
 &\quad + \frac{w}{2} \exp[\mp k\tau] \int_0^1 \frac{T(v, \sigma) d\sigma}{1 \pm k\sigma} .
 \end{aligned}$$

For $w = 1$, the linear constraints are

$$2v(1 - \exp[-\tau/v]) = \int_0^1 [S(v, \sigma) + T(v, \sigma)] d\sigma$$

$$(4.13) \quad \tau \int_0^1 T(v, \sigma) d\sigma = 2v^2 \left(1 - (1 + \tau/v) \exp[-\tau/v] \right) \\ + \int_0^1 \sigma [S(v, \sigma) - T(v, \sigma)] d\sigma$$

In view of (3.11) we expect solutions to (4.11) to be given simply by solutions to (4.10).

Even though (4.10) is important in its relation to scattering and transmission functions, (4.8) for x and $\tau-x$ are equally important since they determine the source function J at any symmetric depths in the slab. Any numerical method for treating (4.10) applies equally well to (4.8). This is of particular significance in reactor criticality problems [37]. In a paper currently being written with Mr. Leonard, we are showing that a study of (4.8) leads both to the criticality condition for slabs and spheres, i.e., the functional relation between τ and the average neutron production per fission, and to Fredholm equations for the neutron density in these critical reactors. This is related to, but simpler than, some current work in neutron transport [21, 45, 48, 80].

Although (4.3) and the resulting equations have been

derived from the transport equation, they express some physical principle of duality. The transport equation, which expresses differential changes in I interior to the slab, has been replaced by an equation which relates J , and hence also I , at x and $\tau-x$ by means of the functional dependence of J on variations of the angle of incident radiation on the face of the atmosphere. We refrain from designating this as a new principle.

5. THE UNIQUENESS PROBLEM

Before considering the merits of various equations for numerical computations it is imperative to determine whether or not each set of equations has a unique solution. For some reason this problem is often confused with the problem of uniqueness in the physical problem supposedly represented by the mathematical model.

We illustrate with a quote from Ambarzumian [3, p. 559], where he is discussing the symmetry of the function S (ρ in his notation) for a semi-infinite atmosphere "... However, since equation (33.24) can have, from its physical significance, only one solution, the function $\rho(r, \xi)$ must be symmetrical: ...".

The conclusion about symmetry reached by this argument is correct. However, the reasoning is incorrect since, except in the conservative case of $w = 1$, the equation he is discussing has two symmetric solutions expressed in terms of the two solutions [16] to Ambarzumian's equation (eqn. (33.28) on p. 559 of [3]) or, what is the same thing, Chandrasekhar's H equation.

We quote from Chandrasekhar [22, p. 208] as an illustration of a more appropriate viewpoint. "The reference to the question of uniqueness of the solution in the preceding paragraph draws attention to a fact which we have so far ignored, namely, that there are, indeed, no grounds for believing that the principles of

invariance, by themselves, can lead to determine solutions of the various problems. The invariances and the equations they lead to are only necessary conditions; it is by no means obvious that they are also sufficient....."

The confusion of physical models with mathematical models often causes the mathematician's query to be termed "academic" when he asks, "But do the equations have a unique solution?" With regard to some of the equations given in previous sections we shall see just how relevant is this question.

Let us consider first the nonlinear equations (3.12) for X and Y functions. Chandrasekhar realized the importance of the uniqueness problem for these equations, and, in fact, he shows [22] that these equations have a one parameter family of solutions for $w = 1$. The uniqueness problem is also considered by Busbridge [16]. We [51] recently gave a complete discussion of the solutions to equations similar to (3.12) but with w replaced under the integral by a nonnegative "characteristic function" whose integral is bounded by $1/2$. We have also studied the uniqueness question for similar equations in anisotropic scattering [52].

For isotropic scattering we show in [51] that for $w = 1$ Chandrasekhar found only half of the solutions to (3.12). We designate by X_0 and Y_0 the functions (3.4). Then all solutions to (3.12) for $w = 1$ are given by

$$(5.1) \quad X(\mu) = (1 + b\gamma\mu)X_0(\mu) + \mu(a+b\mu)[X_0(\mu) + Y_0(\mu)] ,$$

$$Y(\mu) = (1 - b\gamma\mu)Y_0(\mu) - \mu(a - b\mu)[X_0(\mu) + Y_0(\mu)] .$$

The constant γ is given by

$$(5.2) \quad \gamma = \frac{x_1 + y_1}{y_0}$$

with

$$(5.3) \quad x_1 = \frac{1}{2} \int_0^1 X_0(v)v^1 dv , \quad y_1 = \frac{1}{2} \int_0^1 Y_0(v)v^1 dv .$$

The parameters a and b are arbitrary solutions to

$$(5.4) \quad b(b\gamma^2 + 2a\gamma - 2) = 0 .$$

The solutions with $b = 0$ are given by Chandrasekhar [22].

For $0 \leq w < 1$ the solutions to (3.12) are given by

$$\begin{aligned}
 x(\mu) = & \left[1 + \frac{(fa-g\beta)\mu+k\mu^2(fa+g\beta)}{1-(k\mu)^2} \right] x_0(\mu) \\
 & + \frac{(f\beta-g\alpha)\mu+k\mu^2(f\beta+g\alpha)}{1-(k\mu)^2} y_0(\mu) , \\
 (5.5)
 \end{aligned}$$

$$\begin{aligned}
 y(\mu) = & \left[1 - \frac{(fa-g\beta)\mu-k\mu^2(fa+g\beta)}{1-(k\mu)^2} \right] y_0(\mu) \\
 & - \frac{(f\beta-g\alpha)\mu-k\mu^2(f\beta+g\alpha)}{1-(k\mu)^2} x_0(\mu)
 \end{aligned}$$

The constant k is given by (4.5) and constants α and β are given by

$$\alpha = 1 - \frac{w}{2} \int_0^1 \frac{x_0(v)}{1+kv} dv ,$$

(5.6)

$$\beta = \frac{w}{2} \int_0^1 \frac{y_0(v)}{1+kv} dv .$$

The parameters f and g are arbitrary points on the hyperbola

$$(5.7) \quad (f^2-g^2)(\alpha^2-\beta^2) = 2k(fa+g\beta).$$

These results were easily obtained by first describing all solutions to the linear equations (4.10). The totality of such solutions is given either by (5.1) and with arbitrary parameters a and b or by (5.5) and arbitrary parameters f and g . The constraints (5.3) on a and b and (5.6) on f and g are the only additional restriction imposed by the nonlinear equations (3.12).

So we have a set of equations (3.12) which were first derived from heuristic "Invariance Principles". If the variable μ is restricted to the values $0 \leq \mu \leq 1$ of physical interest, these equations alone do not specify a unique solution. It is easily shown that the linear constraints (4.6), evaluated at $x = 0$, are additional equations needed to select the desired functionals, X and Y , of the solution J to (2.6). But it is hardly likely that these constraints would be derived by a heuristic particle counting. They come from the mathematical condition of analyticity in a variable which is usually restricted to the interval $0 \leq \mu \leq 1$ as the cosine of an angle in the interval $[0, \frac{\pi}{2}]$.

The fact that equations (3.12) do not have a unique solution does not mean that they are wrong. It just means that they do not constitute a complete set of equations. Without a mathematical investigation of uniqueness of solution to a set of equations it is not always possible to say that the some needed equations may not have been overlooked.

As we have already remarked, the linear equations (4.10) have a two parameter family of solutions. We know, however, that the constraints (4.6) are also necessary conditions. These constraints and equations (4.10) are a complete set of equations with a unique solution. We shall see in Section 7 that these equations can be transformed to a form ideal for numerical computation.

We have not discussed the uniqueness problem for the nonlinear integro-differential equations (3.13). We shall do this along with other considerations in the next section.

6. INSTABILITY RESULTS

In this section we wish to discuss the appropriateness of the various nonlinear equations for numerical computations. We are particularly interested in the problem of stability. Since solutions to equations are usually approximated by numerical solutions to approximate equations, it is helpful, in bounding errors, to know properties of solutions to the perturbed equations, in particular, their degree of approximation to the solution to the exact equations.

We wish first of all to consider the nonlinear X and Y equations (3.12). To understand the importance for numerical computations of the multiplicity of solutions given in Sec. 5 we need a result about the function J .

Theorem 4. Let $e(\tau)$ denote the maximum eigenvalue of the operator \mathcal{A} . Then $e(\tau) < 1$ for $0 \leq \tau < \infty$, and the solution J to (2.6) is an analytic function of ω for all complex ω in the domain $|\omega| < 1/e(\tau)$.

This theorem is easily established by standard spectral theory arguments about the inverse $(I - \omega \mathcal{A})^{-1}$ for the compact, positive definite, self-adjoint operator \mathcal{A} .

This result shows that the functions X_0 and Y_0 have power series expansions in ω which converge in the circle $|\omega| < 1/e(\tau)$. We now show that this fails to be true for all solutions (5.1) and (5.5) to (3.12) other than X_0 and Y_0 .

The function (5.5) contain the constant k . As a function of ω , k is determined by (4.5), which we rewrite as

$$(6.1) \quad \frac{1-\omega}{\omega} = k^2 \left[\frac{1}{3} + \frac{k^2}{5} + \dots + \frac{k^{2n-2}}{2n+1} \dots \right], \quad |k| < 1.$$

It is easily seen that $k = 1$ at $\omega = 0$, but that k as a function of complex ω has a singularity at $\omega = 0$ and a branch point of order 2 at $\omega = 1$. Therefore k in (5.5) is not an analytic function of ω even in the domain $|\omega| < 1$. The functions given in (5.1) are appropriate limits of those given in (5.5) as ω tends to 1 and k tends to 0, where k has a branch point as a function of ω .

We obtain then another characterization of the functions X_0 and Y_0 .

Theorem 5. There is a unique solution to equations (3.12) which is analytic in ω for $|\omega| < 1/e(\tau)$, namely the functions X_0 and Y_0 .

A standard numerical technique for solving functional equations such as (3.12) is by iteration [3, 20, 26, 27, 32, 61]. Let the iterations be defined by

$$\begin{aligned}
 (6.2) \quad X_{n+1}(\mu) &= 1 + \frac{\mu\omega}{2} \int_0^1 \frac{X_n(\mu)X_n(\nu) - Y_n(\mu)Y_n(\nu)}{\mu + \nu} d\nu, \\
 Y_{n+1}(\mu) &= \exp[-\tau/\mu] + \frac{\mu\omega}{2} \int_0^1 \frac{Y_n(\mu)X_n(\nu) - X_n(\mu)Y_n(\nu)}{\mu - \nu} d\nu,
 \end{aligned}$$

$$X_1 = Y_1 = 0.$$

This generates the n -th partial sums in the power series expansion of the solutions X_0 and Y_0 . This procedure is also equivalent to introducing in (3.12) the power series expansions in powers of ω and equating coefficients, a standard perturbation analysis.

By Theorem 5 this iterative method, if computed with absolute precision, leads to the desired solution X_0 and Y_0 to (3.12) by reason of the analyticity. But what of the many solutions (5.1) or (5.5)? These are solutions to (3.12) which are not analytic in ω and in theory will not be reached by the iterative method as long as the initial functions in the iteration are not chosen to be one of these extraneous solutions.

There are, however, extraneous solutions to (3.12) which are arbitrarily close to the desired solution (X_0, Y_0) . It is to be expected, as has been observed, that as the iterations seem to be converging, numerical errors introduce the influence of the extraneous solutions and cause oscillations. So in theory the iterative methods

will converge to a unique solution, but in practice the presence of extraneous solutions arbitrarily near the limit introduces instability in the calculations. Only by extreme accuracy can this instability be avoided in treating the X and Y equations (3.12).

The nonlinear equations (3.12) are obtained from (3.9) without any use of (3.10). This results in nonuniqueness of solutions. Rather than consider (3.9) and (3.10) we now consider the equation (3.13) for the function S . This is a nonlinear integro-differential equation for determining S as a function of the total optical thickness τ of the atmosphere. The initial condition on S for $\tau = 0$, i.e., no atmosphere, is naturally

$$(6.3) \quad S(\mu, \mu_0, 0) = 0 .$$

Equations (3.13) and (6.3) represent the conversion of a boundary value problem for linear equations (2.1) and (2.3) to an initial value problem for Ricatti type equations. The computational advantage of such a formulation is obvious and has been much emphasized [13, 63]. Computations with these equations have been performed for isotropic scattering [14].

If we specify an initial function for S at $\tau = \tau_0$ by

$$(6.4) \quad S(\mu, \nu, \tau_0) = s(\mu, \nu) ,$$

we can readily convert (3.13) to a nonlinear integral equation of Volterra type

$$\begin{aligned}
 (6.5) \quad S(\mu, \nu, \tau) = & \exp\left[\frac{\mu\nu(\tau-\tau_0)}{\mu+\nu}\right] s(\mu, \nu) + \int_{\tau_0}^{\tau} \exp\left[\frac{-\mu\nu(\tau-t)}{\mu+\nu}\right] \times \\
 & \times \left[1 + \frac{\omega}{2} \int_0^1 S(\mu, \sigma, t) \frac{d\sigma}{\sigma}\right] \left[1 + \frac{\omega}{2} \int_0^1 S(\nu, \sigma, t) \frac{d\sigma}{\sigma}\right] dt.
 \end{aligned}$$

One can show that for sufficiently small $\tau - \tau_0$ and s the right hand side of (6.5) is a contracting operator and, hence, that the equation has a unique solution.

This solution can be continued for larger values of τ .

In recent reports [55, 56] we have studied solutions to (3.13) and a family of initial conditions (6.4). This is actually equivalent to studying equations (3.14) and (3.15). Of particular interest are a family of singular solutions, i.e., infinite for finite τ , and their nearness of approach to the desired solution for increasing τ .

We designate the solution to (3.13) and (6.3) by S_0 . It can be shown that

$$(6.6) \quad \lim_{\tau \rightarrow \infty} S_0(\mu, \nu, \tau) = \frac{\mu\nu}{\mu+\nu} H(\mu)H(\nu),$$

where H is Chandrasekhar's notation (see also Ambarzumian [3]) for the limiting value of the function X_0 as τ tends to infinity.

We consider first the conservative case, i.e., $w = 1$. It can be shown [51, 53, 55] that as τ tends to infinity

$$(6.7) \quad S_0(\mu, \nu, \tau) = \frac{\mu\nu}{\mu+\nu} H(\mu)H(\nu) + O\left(\frac{1}{\tau}\right).$$

So S_0 approaches the limit, given in (6.6), only as $1/\tau$.

By use of (3.14) and (3.15) and (5.1) - (5.3) it is possible to exhibit solutions to (3.13) and initial conditions

$$(6.8) \quad S(\mu, \nu, 0) = 4(1 + 2 B\mu\nu)\mu\nu.$$

We have given explicit solutions for (6.8)[55], but we only give them here in the form

$$S(\mu, \nu, \tau) = S_0(\mu, \nu, \tau) + O\left(\frac{1}{\tau}\right) + \frac{B}{1 - 2B \int_0^\tau (x_1(t) + y_1(t))^2 dt} O(1)$$

For any $B > 0$ these solutions are infinite for some finite value of τ . By choosing B sufficiently small and positive and τ sufficiently large it is possible to find a singular solution which comes arbitrarily close to the solution S_0 before it becomes infinite.

For $0 \leq \omega < 1$ there are also singular solutions to (3.13), but then these can come within a distance of S_0 proportional to the constant k and no closer. Since the initial conditions and solutions are more complicated in this case, we merely refer to [56] for details.

The nonlinear integrodifferential equations with initial conditions are attractive from the numerical viewpoint. The above results show, however, that there is a limit to the accuracy which can be achieved for large values of τ , at least in the conservative and near-conservative cases.

7. LINEAR FREDHOLM EQUATIONS

We conclude with a quick survey of some results obtained from the linear singular equations (4.10) and linear constraints (4.6) or (4.7). The method for treating these equations is to invert the singular operator. By analytic continuation the transformed equations can then be transformed to Fredholm equations with continuous kernels. The same program has been carried out for anisotropic scattering [54], but in less complete form.

For simplicity we merely give here the results for $\omega = 1$. Complete details are given in [53] for X and Y equations with a characteristic function ψ instead of the constant ω , and in [54] for anisotropic scattering. The equations for X and Y functions have been programmed.

By consistent use of the theory of singular integral equations and analytic function theory, we have obtained the following formulae.

We designate by H the limit of the X_0 function as τ tends to infinity. Then H is given on $0 \leq \mu \leq 1$ by the formula [53]

$$(7.1) \quad H(\mu) = (1+\mu) \exp \left[\mu \int_0^1 \frac{\theta(t)}{t(t+\mu)} dt \right]$$

The function λ_0 is given by (4.9) for $\omega = 1$, and θ is defined by

$$(7.2) \quad \theta(\mu) = \frac{1}{\pi} \tan^{-1} \left[\frac{\pi\mu}{2\lambda_0(\mu)} \right], \quad 0 \leq \theta \leq 1.$$

The formula (7.1) is not given in [53] but is obtained from the formula given there by analytic continuation.

For finite values of τ we obtain X_0 and Y_0 functions as corrections to (7.1). We have [53]

$$(7.3) \quad X_0(\mu) = H(\mu) \left\{ f(\mu) - \mu \exp \left[\int_0^1 \frac{\theta(t)}{t} dt \right] \frac{1 - \int_0^1 \theta(t) dt}{\tau + 2 \left(1 - \int_0^1 \theta(t) dt \right)} \right. \\ \left. + \frac{\mu}{2} \int_0^1 \frac{f(t) - f(\mu)}{t - \mu} \frac{dt}{H(t) \left([\lambda_0(t)]^2 + \left[\frac{\pi t}{2} \right]^2 \right)^{1/2}} \right\},$$

and

$$(7.4) \quad Y_0(\mu) = H(\mu) \left\{ g(\mu) + \mu \exp \left[\int_0^1 \frac{\theta(t)}{t} dt \right] \left(\frac{1 - \int_0^1 \theta(t) dt}{\tau + 2 \left(1 - \int_0^1 \theta(t) dt \right)} - 1 \right) \right. \\ \left. + \frac{\mu}{2} \int_0^1 \frac{g(t) - g(\mu)}{t - \mu} \frac{dt}{H(t) \left([\lambda_0(t)]^2 + \left[\frac{\pi t}{2} \right]^2 \right)^{1/2}} \right\}.$$

The functions f and g are given by

$$(7.5) \quad f = \frac{P+Q}{2}, \quad g = \frac{P-Q}{2},$$

where P and Q satisfy the Fredholm equations

$$(7.6) \quad P = -L(P) + 1 + \exp[-\tau/\mu](1 - \mu N(-\mu)),$$

$$Q = L(Q) + 1 - \exp[-\tau/\mu] \left(1 - \frac{\mu \tau N(-\mu)}{\tau + 2 \left(1 - \int_0^1 \theta(t) dt \right)} \right),$$

with

$$(7.7) \quad N(-\mu) = \frac{\exp \left[\int_0^1 \frac{\theta(t)}{t + \mu} dt \right]}{1 + \mu}.$$

The linear integral operator L , which we shall not display, has a continuous nonnegative kernel. The equations (7.6) can be solved by iteration to converge uniformly, since, in this norm, we have shown [53] that

$$(7.8) \quad ||L|| \leq \left(1 - \exp \left[\int_0^1 \frac{\theta(t)}{t} dt \right] \right) e^{-\tau}.$$

The convergence is very rapid except for τ near 0.

A numerical program for computing X_0 and Y_0 from these formulae has a natural check. For $\tau = 0$ the computations are no different than for $\tau > 0$ and must generate X_0 and Y_0 to be identically 1. This amounts to computing H by (7.1) and then generating $1/H$ by the formula

$$(7.9) \quad H^{-1}(\mu) = f(\mu) - \frac{\mu}{2} \exp \left[\int_0^1 \frac{\theta(t)}{t} dt \right] \\ + \frac{\mu}{2} \int_0^1 \frac{f(t) - f(\mu)}{t - \mu} \frac{dt}{H(t) \left([\lambda_0(t)]^2 + [\frac{\pi t}{2}]^2 \right)^{1/2}},$$

where now

$$(7.10) \quad f = -L(f) + 1 - \frac{\mu}{2(1+\mu)} \exp \left[\int_0^1 \frac{\theta(t)}{t + \mu} dt \right].$$

We see then that the linear equations and linear constraints have a unique solution. By the use of analytic function theory these are reduced to quadratures and rapidly convergent Fredholm equations.

8. CONCLUSION

We have surveyed various nonlinear and linear equations as possible substitutes for the Neumann series solution of the transport equation. We have tried not to forget the motivation for studying these equations, that of producing a simpler computation than the Neumann series.

The details that we have been able to give are possible because of the existence of exact linear equations among whose solutions are all the solutions to the nonlinear equations. We have been able to give existence and uniqueness results as well as results relevant to the stability problem for numerical computations. This wealth of detail is primarily a result of the assumption of homogeneity of the atmosphere. All of the results have been [52,54], or can readily be, extended to the anisotropic but homogeneous atmosphere.

We will not rate the various numerical methods. Since we have made no estimates on the rate of convergence of iterative methods for nonlinear equations, it is not possible to compare them with the computations based on the linear Fredholm equations. Nor have we given any quantitative measure of the seriousness of the instabilities discussed in Sec. 6. We have shown that instabilities put bounds on the accuracy of numerical computations in certain cases. But it may be that

satisfactory accuracy can be attained before instability sets in [14].

As we have remarked before, the linear singular equations are a result of the assumption of homogeneity, as clarified in Sec. 2. Numerical methods for solving equations (3.13) or equations (3.14) and (3.15) perhaps have the greatest potential since analogous equations can be formulated for inhomogeneous problems [10,19,74]. The detailed analysis of the linear equations for homogeneous problems and the ensuing results for nonlinear equations is of value, if for no other reason, in giving indications of behavior to be expected in a study of the more complicated inhomogeneous problems.

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